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chain nodes :
7 8 9 10 11 12
ring nodes :
1 2 3 4 5 6
chain bonds :
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ring bonds :
1-6 1-2 2-3 3-4 4-5 5-6
exact/norm bonds :
4-7 7-8 8-9 9-10 10-11
normalized bonds :
1-6 1-2 2-3 3-4 4-5 5-6
isolated ring systems :
containing 1 :
Match level :
1:CLASS 2:CLASS 3:CLASS 4:CLASS 5:CLASS 6:CLASS 7:CLASS 8:CLASS 9:CLASS
10:CLASS 11:CLASS 12:CLASS 14:CLASS
Generic attributes :
11:
Saturation
                      : Unsaturated
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : Exactly 1
Type of Ring System : Monocyclic
12:
Number of Carbon Atoms : less than 7
Number of Hetero Atoms : 2 or more
Type of Ring System : Monocyclic
Element Count :
Node 11: Limited
   C,C5
   N,N1
Node 12: Limited
   C,C3
   0,01
   N,N1
   S,SO
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L1

L1

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L2 0 SEA SSS SAM L1

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33 SEA SSS FUL L1 L3

=> s 13 and caplus/lc 59456180 CAPLUS/LC

32 L3 AND CAPLUS/LC

=> s 13 not 14

1 L3 NOT L4 L5

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0 ANSWERS

33 ANSWERS

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L5 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2008 ACS on STN RN 794492-66-3 REGISTRY ED Entered STN: 08 Dec 2004 CN 4-Pyridineacetic acid, α-[2-[4-(5-oxazolyl)phenyl]hydrazinylidene]-, (α2)- (CA INDEX NAME) CTHER CA INDEX NAMES: CN 4-Pyridineacetic acid, α-[[4-(5-oxazolyl)phenyl]hydrazono]-, (α2)- (9C1) FS STEREOSEARCH MF C16 H12 N4 O3 CI CCM SR CA
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Double bond geometry as shown.

PROPERTY DATA AVAILABLE IN THE 'PROP' FORMAT

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FULL ESTIMATED COST

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L1 STRUCTURE UPLOADED

L2 0 S L1

L3 33 S L1 FULL

L4 32 S L3 AND CAPLUS/LC

L5 1 S L3 NOT L4

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=> s 14

L6 2 L4

=> d ibib abs hitstr 1-2

L6 ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN ACCESSION NUMBER: 2007:1390731 CAPLUS DOCUMENT NUMBER: 148:158944

TITLE:

148:158944
Orally administered amyloidophilic compounds is effective in prolonging the incubation periods of animals cerebrally infected with prion diseases in a prion strain-dependent manner Kawasaki, Yuri; Kawagoe, Keichi; Chen, Chun-jen; Teruya, Kenta; Sakaegawa, Yuji; Doh-ura, Katsumi Department of Frion Research, Tohoku University Graduate School of Medicine, Sendai, Japan Journal of Virology (2007), 81(23), 12889-12898 CODEN: JOUYAN; ISSN: 0022-538 American Society for Microbiology Journal AUTHOR(S): CORPORATE SOURCE: SOURCE:

DIEBLISHER.

PUBLISHER: American Society for Microbiology
DOCUMENT TYPE: Journal
LANGUAGE: English
AB The establishment of effective therapeutic interventions for prion
diseases is necessary. We report on a newly developed amyloidophilic
compound that displays therapeutic efficacy when administered orally.
Thie

compound inhibited abnormal prion protein formation in prion-infected neuroblastoma cells in a prion strain-dependent manner: effectively for RML prion and marginally for 22L prion and Fukuoka-1 prion. When the highest dose (0.2% kmt/wt] in feed) was given orally to cerebrally RML prion-inoculated mice from inoculation until the terminal stage of disease, it extended the incubation periods by 2.3 times compared to the control. The compound exerted therapeutic efficacy in a prion strain-dependent manner such as that observed in the cell culture study:

effective for RML prion, less effective for 22L prion or Fukuoka-1 prion, and marginally effective for 263K prion. Its effectiveness depended on

earlier start of administration. The glycoform pattern of the abnormal prion protein in the treated mice was modified and showed predominance of the diglycosylated form, which resembled that of 263% prion, suggesting that diglycosylated forms of abnormal prion protein might be least sensitive or resistant to the compound The mechanism of the prion strain-dependent effectiveness needs to be elucidated and managed. Nevertheless, the identification of an orally available amyloidophilic chemical encourages the pursuit of chemotherapy for prion diseases. 774236-55-4

774236-55-4
RL: PAC (Pharmacological activity); PKT (Pharmacokinetics); THU (Therapeutic use); BIOL (Biological study); USES (Uses) (orally administered amyloidophilic compds. are effective in

prolonging nging the incubation periods of animals cerebrally infected with prion diseases in a prion strain-dependent manner) 774236-55-4 CAPLUS

4-Pyridinecarboxaldehyde, 2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN
ACCESSION NUMBER: 2004:857547 CAPLUS
DOCUMENT NUMBER: 414:335174 CAPLUS
1111.35174 Preparation of benzaldehyde or heterocycle carboxaldehyde hydrazone derivatives as inhibitors of agglutination and/or deposition of an amyloid protein or amyloid-like protein
INVENTOR(S): Kawagoe, Reiichi; Motoki; Kayoko; Odagiri, Takashi; Suzuki, Nobuyuki; Chen, Chun-Jen; Mimura, Tetsuya
PATENT ASSIGNEE(S): Daiichi Fharmaceutical Co., Ltd., Japan
SOURCE: PCT Int. Appl., 236 pp.
CODEN: PIXXD2
DOCUMENT TYPE: Patent
LANGUAGE: Japanese

Japanese

LANGUAGE: FAMILY ACC. NUM. COUNT: PATENT INFORMATION:

PATENT NO. KIND DATE APPLICATION NO. DATE WO 2004087641 A1 20041014 WO 2004-JP4607 20040331 TD. TG A1 20041014 CA 2004-2521056 20040331 CA 2521056 R: AT, BE, CH, DE, DK, ES, FK, GB, GR, IT, LI, LU, NL, SE, MC, PT, IE, SI, LT, LV, FI, RO, MK, CY, AL, TR, BG, CZ, EE, HU, PL, SK US 20060276433 A1 20061207 US 2005-551414 20050930 JP 2003-94257 A 20030333 PRIORITY APPLN. INFO.: WO 2004-JP4607 W 20040331

OTHER SOURCE(S): MARPAT 141:350174

 $\sum_{R^2}^{R^1} N - N - Ar - X - G$

Compds. represented by the general formula (I), salts thereof, or

AB Compds. represented by the general formula (1), salts thereot, or solvates solvates of either [R1, R2 = H, alkyl, alkenyl, alkynyl, aralkyl, NH2, alkylamino, cyano, halo, haloalkyl, haloalkynyl, haloalkynyl, CONH2, N-alkylcarbamoyl, N.N-dialkylcarbamoyl, N-hydroxyalkylcarbamoyl, each (un)substituted aryl, (un)saturated 5- to 7-membered heterocyclyl, (un)saturated bi- or tricyclic condensed heterocyclyl alkenyl, or un)saturated bi- or tricyclic condensed heterocyclylalkenyl, or un)saturated bi- or tricyclic condensed

heterocyclylalkenyl, or (un)saturated bi- or tricyclic condensed

ANSWER 1 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



REFERENCE COUNT:

32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR

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ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) heterocyclylalkenyl,R3 = H, (un)substituted alkyl, acyl, alkoxycarbonyl; Ar = a divalent group derived from arom. hydrocarbon, (un)satd. 5- to 7-membered heterocyclic group, or (un)satd. bi- or tricyclic condensed heterocyclic group; X = a single bond, a single bond, each substituted linear or branched C1-3 alkylene, C1-3 alkenylene, or C1-3 alkynylene,

G = halo, haloalkyl, haloalkenyl, haloalkynyl, alkoxy, alkoxycarbonyl, N-alkylamino, N,N-dialkylamino, each (un)substituted (un)satd. bi- or tricyclic condensed hydrocarbyl, (un)satd. 5- to 7-membered heterocyclyl, or (un)satd. bi- or tricyclic heterocyclyl] are prept. Also disclosed is (1) an agent for inhibiting the agglutination and/or deposition of an amyloid protein or amyloid-like protein or (2) a preventive and/or remedy for conformational diseases or diseases caused by amyloid accumulation, which contains the compd. I, its salt, or solvate thereof. In igular. particular,

which contains the compd. 1, its sait, or solvate thereof. In ioular, disclosed is a preventive and/or remedy for Alzheimer's disease, Down's syndrome, Creutzfeldt-Jakob disease, type II diabetes, dialysis amyloidosis, AA amyloidosis, Gerstmann-Straussler-Scheinker (GSS) syndrome, Muckle-Wells syndrome, localized atrial amyloidosis, thyroid medullary carcinoma, skin amyloidosis, localized tuberous amyloidosis, AI amyloidosis, AH amyloidosis, Familal Mediterranean fever, Parkinson's disease, tauopathy, ALS, or CAG repeat disease. A radiodiagnostic agent contg. radionuclide-labeled, in particular radioactive iodine-labeled compd. I is also disclosed. Thus, 1.0 g 4-(oxazol-5-yl)phenylhydrazine and 0.61 g 4-pyridinecarboxaldehyde were heated in ethanol at reflux overnight to give, after recrystn. from ethanol, 1.03 g 4-pyridinecarboxaldehyde N-[4-(oxazol-5-yl)phenyl)hydrazone (II). II inhibited the formation of amyloid from amyloid β protein with IC50 of 2.94 μM vs. 0.87 and 3.23 μM for Cogo Red and 2-(1,1-dicyanopropen-2-yl)-6-dimethylaminonaphthalene (DDNP), resp. 774236-55-4P

774236-55-4P

//4236-50-4P RE: FAC (Pharmacological activity); RCT (Reactant); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); RACT (Reactant or reagent); USES (Uses) (preparation of benzaldehyde or heterocycle carboxaldehyde hydrazone

as inhibitors of agglutination and/or deposition of amyloid protein or amyloid-like protein) 774236-55-4 CAPLUS

,,4230-33-4 CAPLUS 4-Pyridinecarboxaldehyde, 2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

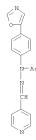
774236-56-5P 774236-57-6P 774236-58-7P
774236-59-8P 774236-60-1P 774236-61-2P
774236-62-3P 774236-80-5P 774236-61-2P
774236-5-8P 774236-80-5P 774236-83-8P
774236-91-8P 774236-92-9P 774237-28-4P
774237-39-5P 774237-34-2P 774237-35-3P
774237-36-4P 774237-37-5P 774237-6-P
774237-78-2P 774237-78-9-8P 774237-70-6P
774237-78-5P 774237-78-9-8P 774237-81-9P
774237-68-4P
RL: PRC (Pharmacological activity); SPN (Synthetic preparation); THU (Therapeutic use); BIOL (Biological study); PREF (Preparation); USES (Uses)
(preparation of benzaldehyde or heterocycle carboxaldehyde hydrazo

(USES)
(preparation of benzaldehyde or heterocycle carboxaldehyde hydrazone derivs.

vs.

as inhibitors of agglutination and/or deposition of amyloid protein or
amyloid-like protein)
774236-56-5 CAPLUS
Hydrazinecarboxylic acid, 1-[4-(5-oxazolyl)phenyl]-2-(4pyridinylmethylene)-, 1,1-dimethylethyl ester (CA INDEX NAME)

774236-57-6 CAPLUS Acetic acid, 1-[4-(5-oxazoly1)pheny1]-2-(4-pyridinylmethylene)hydrazide (CA INDEX NAME)



774236-58-7 CAPLUS 4-Pyridinecarboxaldehyde, 2-methyl-2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

774236-59-8 CAPLUS
Bydrazinecarboxylic acid, 1-[4-(4-iodo-5-oxazolyl)phenyl]-2-(4pyridinylmethylene)-, 1,1-dimethylethyl ester (CA INDEX NAME)

774236-60-1 CAPLUS //420-00-1 CAFBOS 4-Pyridinecarboxaldehyde, 2-[4-(4-iodo-5-oxazolyl)phenyl]hydrazone (CA INDEX NAME) ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

774236-61-2 CAPLUS
4-Pyridinecarboxaldehyde, 2-[3-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

774236-62-3 CAPLUS
4-Pyridinecarboxaldehyde, 2-[2-(5-oxazoly1)pheny1]hydrazone (CA INDEX NAME)

RN 774236-70-3 CAPLUS
CN Hydrazinecarboxylic acid,
1-[4-[4-(hydroxymethyl)-5-oxazolyl]phenyl]-2-(4pyridinylmethylene)-, 1,1-dimethylethyl ester (CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

774236-71-4 CAPLUS
4-Pyridinecarboxaldehyde, 2-[4-[4-(hydroxymethyl)-5-oxazolyl]phenyl]hydrazone (CA INDEX NAME)

RN CN

774236-75-8 CAPLUS
4-Pyridinecarboxaldehyde, 2-[4-(4,5-dihydro-2-oxazolyl)phenyl]hydrazone
(CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)



774236-92-9 CAPLUS 3-Pyridinecarboxaldehyde, 2-[4-(5-oxazoly1)pheny1]hydrazone (CA INDEX NAME)

774237-28-4 CAPLUS 4-Pyridinecarboxaldehyde, 2-[2-iodo-4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued) 774236-80-5 CAPLUS Methanone, phenyl-4-pyridinyl-, 2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

774236-83-8 CAPLUS Ethanone, 1-(4-pyridiny1)-, 2-[4-(5-oxazoly1)phenyl]hydrazone (CA INDEX NAME)

774236-91-8 CAPLUS 2-Pyridinecarboxaldehyde, 2-[4-(5-oxazoly1)phenyl]hydrazone (CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

774237-29-5 CAPLUS
4-Pyridinecarboxaldehyde, 2-[3-iodo-4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

774237-34-2 CAPLUS 4-Pyridinecarboxaldehyde, 3-iodo-, 2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NABL)

774237-35-3 CAPLUS 4-Pyridinecarboxaldehyde, 2-iodo-, 2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

774237-36-4 CAPLUS 4-Pyridinecarboxaldehyde, 2-fluoro-, 2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

RN

774237-68-2 CAPLUS
3-Pyridinecarboxaldehyde, 6-fluoro-, 2-[4-(5-oxazoly1)phenyl]hydrazone (CA INDEX NAME) CN

774237-69-3 CAPLUS
3-Pyridinecarboxaldehyde, 6-(4-methyl-1-piperazinyl)-,
2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

774237-37-5 CAPLUS
4-Pyridinecarboxaldehyde, 2-(4-methyl-1-piperazinyl)-,
2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

774237-67-1 CAPLUS 4-Pyridinecarboxaldehyde, 2-(dimethylamino)-, 2-[4-(5-oxazoly1)phenyl]hydrazone (CA INDEX NAME)

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

(Continued) PAGE 1-A

(Continued)



PAGE 2-A



774237-70-6 CAPLUS 3-Pyridinecarboxaldehyde, 6-(dimethylamino)-, 2-[4-(5-oxazoly1)phenyl]hydrazone (CA INDEX NAME)

774237-74-0 CAPLUS
4-Pyridinecarboxaldehyde, 1,2,3,6-tetrahydro-1-(phenylmethyl)-,
2-[4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)

Double bond geometry as shown.

774237-77-3 CAPLUS 4-Pyridineacetic acid, α -[2-[4-(5-oxazolyl)phenyl]hydrazinylidene]-, ethyl ester, (α Z)- (CA INDEX NAME)

(Continued)

ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN

774237-80-8 CAPLUS 4-Pyridineacetamide, N-(2-hydroxyethyl)- α -[2-[4-(5-oxazolyl)phenyl]hydrazinylidene]-, (α Z)- (CA INDEX NAME)

Double bond geometry as shown.

774237-81-9 CAPLUS 4-Pyridinecarbohydrazonoyl chloride, N-[4-(5-oxazolyl)phenyl]- (CA INDEX NAME)

774237-78-4 CAPLUS 4-Pyridineacetic acid, α -[2-[4-(5-oxazolyl)phenyl]hydrazinylidene]-, hydrochloride (1:1), (α Z)- (CA INDEX NAME)

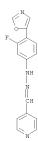
Double bond geometry as shown.

• HCl

774237-79-5 CAPLUS 4-Pyridineacetamide, α -[2-[4-(5-oxazoly1)phenyl]hydrazinylidene]-(CA INDEX NAME)

L6 ANSWER 2 OF 2 CAPLUS COPYRIGHT 2008 ACS on STN (Continued)

774237-86-4 CAPLUS
4-Pyridinecarboxaldehyde, 2-[3-fluoro-4-(5-oxazolyl)phenyl]hydrazone (CA INDEX NAME)



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